

# Structural transitions in a classical two-dimensional molecule system

W. P. Ferreira<sup>1</sup>, G. A. Farias<sup>1</sup>, H. A. Carmona<sup>2</sup>, and F. M. Peeters<sup>3</sup>

<sup>1</sup>*Departamento de Física, Universidade Federal do Ceará, Caixa Postal 6030,  
Campus do Pici, 60455-760 Fortaleza, Ceará, Brazil.*

<sup>2</sup>*Departamento de Física e Química, Universidade Estadual do Ceará, Av. Paranjana, 1700  
Fortaleza, Ceará, Brazil.*

<sup>3</sup>*Departement Natuurkunde, Universiteit Antwerpen (UIA), Universiteitsplein 1, B-2610  
Antwerpen, Belgium*

(February 1, 2008)

## Abstract

The ground state of a classical two-dimensional (2D) system with a finite number of charges particles, trapped by two positive impurity charges localized at a distance ( $z_0$ ) from the 2D plane and separated from each other by a distance  $x_p$  are obtained. The impurities are allowed to carry more than one positive charge. This classical system can form a 2D-like classical molecule that exhibits *structural transitions* and *spontaneous symmetry breaking* as function of the separation between the positive charges before it transforms into two 2D-like classical atoms. We also observe structural transitions as a function of the dielectric constant of the substrate which supports the charged particles, in addition to broken symmetry states and *unbinding of particles*.

Keywords: Phase transitions, low dimensions , classical molecule

36.40.Ei, 64.60.-i

Typeset using REVTeX

## I. INTRODUCTION

Classical charged particles confined in a two-dimensional (2D) layer has been a subject of interest in the last few years. [1–7] It is well-known that classical 2D electrons form a Wigner crystal. [1,8] On the other hand, confined charged particles in 2D form 2D-like classical atoms [9] which can exhibit very different melting and structural phase transitions. [10] Recently these properties were studied for a set of charged particles confined by a parabolic and hard-wall well. [9–12] They order in a ring structure and a Mendeleev table for these atomic like structures was constructed. An essentially different confinement is the one produced by a Coulomb potential. 2D charges which are confined by this potential also form 2D-like classical atomic structures but they exhibit very different structural transitions as compared to the one confined by parabolic potentials. [13]

In the present paper we extend our previous work for single classical atoms [9,13] and vertically coupled atoms [14] to laterally coupled atoms which form molecular structures. The system we consider here is composed of classical charged point particles interacting through a repulsive Coulomb potential and held together by two remote impurities a distance  $d$  away from the 2D plane where the charged particles can move. The ground state of the system is calculated by using the Monte Carlo simulation technique and by minimization techniques. We show that the ground state of this 2D-like classical molecule (2DCM) presents structural phase transitions and if the impurities are separated further apart it is broken into two 2D-like classical atoms (2DCA). Spontaneous broken symmetry and evaporation is observed, which depend strongly on the effective impurity charges and the distance between them.

## II. THEORETICAL MODEL

Our model consists of a finite number of particles  $N$ , each of them with negative charge  $e = -|e|$ , which move in a 2D plane. Two fixed impurities, each of them with charge  $+Ze$ , are localized a distance  $z_o$  from the 2D plane and are separated by a distance  $X_P$  along

the  $x$ -axis and are placed inside a medium with dielectric constant  $\epsilon$ . All particles interact through a Coulomb potential (see Fig. 1). The energy for such a classical system is given by

$$E = \frac{-Ze^2}{\epsilon} \sum_{i=1}^N \sum_{j=1}^2 \frac{1}{|\vec{R}_i - \vec{D}_j|} + \frac{e^2}{\epsilon_o} \sum_{j>i=1}^N \frac{1}{|\vec{R}_i - \vec{R}_j|}, \quad (1)$$

where  $\vec{R}_i$  is the position of the  $i^{th}$  negative particle at the  $(X, Y)$  plane and  $\vec{D}_j = D_x \vec{e}_x - Z_o \vec{e}_z$  ( $D_x = X_p/2$ ) is the position of the  $j^{th}$  positive charge, *i.e.* the impurity. To keep the problem as simple as possible we have neglected in Eq. (1) the effects due to the image charges. Following our previous work [13] we will vary the dielectric constant  $\epsilon$  through which it is possible to change the effective confinement potential in a continuous way. For convenience, we express the energy in units of  $E_o = e^2/\epsilon_o z_0$  where  $\epsilon_o$  is the dielectric constant of vacuum and all the distances are now in units of  $z_0$ . This reduces Eq. (1) to

$$E^* = \frac{-Z^*}{\epsilon} \sum_{i=1}^N \sum_{j=1}^2 \frac{1}{|\vec{r}_i - \vec{d}_j|} + \sum_{j>i=1}^N \frac{1}{|\vec{r}_i - \vec{r}_j|}, \quad (2)$$

where  $E^* = E/E_o$ ,  $Z^* = Z/\epsilon^*$ ,  $x_p = X_p/z_0$ ,  $\vec{d}_j = \vec{D}_j/z_0$ ,  $\vec{r}_j = \vec{R}_j/z_0$ ,  $\epsilon^* = \epsilon/\epsilon_o$ . In order to obtain the minimum energy configuration we perform a numerical minimization of Eq. (2) with respect to the  $2N$  variables (coordinates  $(x, y)$  of the negative particles).

### III. RESULTS

To perform the numerical simulation, we start from a random distribution of negative particles and obtain the minimum energy configuration by using standard minimization techniques. Next we change, *e.g.*  $x_p$ , slightly and take as the initial configuration the last minimum obtained by our numerical minimization. To have an independent check we also use the Monte Carlo simulation technique starting from several different initial configurations. Different from the results obtained with the 2D classical atom [13] we found that bounded configurations, *i.e.*,  $r_i < \infty \forall i$ , can exist if the total effective charge  $Z_T = 2Z^*$  satisfies the condition  $Z_T \leq N - 1$  for  $N > 1$ . In fact, we observed that the condition for bounded

configurations tends to behave as a single 2-D classical atom, if the distance between the two positive charges goes to zero. To analyze the molecule-atom transition we fix the value of the dielectric constant  $\epsilon^* = 1$ , we consider a system of six electrons and put the two positive charges at the points  $(d_x, 0, -1)$  and  $(-d_x, 0, -1)$ , each with a charge  $Z = 3$ . In Fig. 2 we show the distance  $r_i$  of the six negative particles to the point  $(x, y, z) = (0, 0, 0)$  in the minimum energy configuration as a function of the distance between the positive charges  $x_p = 2d_x$ . We clearly observe four distinct regions. In the first region (I),  $x_p$  is very small and the negative particles are arranged in two equilateral triangles, inside each other (see Fig. 3(a)). The two positive charges (their positions are indicated by the crosses in Fig. 3) are so close to each other that they behave as one central charge. This configuration is very different from the one which was found in the case of a parabolic confinement potential [9] where one particle would be at  $(x,y)=(0,0)$  and the other 5 in a ring around it. At  $x_p = 0.0884$  the system undergoes a small structural transition to region (II)(see Fig. 3(b)) which is of first order. Note that increasing  $x_p$  from  $x_p = 0$  acts as a symmetry breaking field which breaks the rotational symmetry of the configuration depicted in Fig. 3(a). With increasing  $x_p$ , the ground state configuration changes continuously up to  $x_p = 1.0074$  where it undergoes a structural transition and a new configuration appears in region (III). This transition is characterized by the fact that the particles change their positions abruptly (compare solid (II) and open (III) symbols in Fig. 3(c)). With further increase of  $x_p$  the system exhibits a new structural transition to region (IV) at  $x_p = 1.8792$  where the configuration clearly exhibits now inversion symmetry with respect to the center of the coordinate system. In region (IV) the negative particles tend to stay in two triangles, each one close to one of the positive charges. Up to this region, the system behaves as a classical molecule. Namely, all distances between the negative particles are related to the positions of both positive charges. Finally, for a value  $x_p \simeq 3.0$  we observe more explicitly that the negative particles split in two sets, each one correlated to one positive charge. No structural transition is associated with this behavior but, up to this point, the system behaves as two independent 2D classical atoms. This can be seen by the fact that, up to  $x_p \simeq 3.0$  the system exhibits rotational

symmetry along the  $z$ -axis for each of the two positive charges. Different from the structural transition from regions (I) up to (IV), the one from 2D classical molecule to 2D classical atom is not characterized by a structural transition, i.e. it is continuous. In order to visualize these stable states, in Fig. 3 we show typical configurations of the system in each region and in Fig. 4 we plot the distance of three negative particles related to each positive charge. As shown in Fig. 4, when  $x_p \geq 3.0$  the system behaves as two independent atoms, with the negative particles in two equilateral triangles and the positive charges in the center of each one, with energy  $E_{single} \rightarrow -4.899$ . In order to show the order of the structural transitions we calculated the first of the energy as a function of  $x_p$ , by numerically differentiating the energy curve. The results for the first derivative are presented in Fig. 5. As can be seen the first derivative is discontinuous at the structural transitions (I  $\rightarrow$  II, II  $\rightarrow$  III and III  $\rightarrow$  IV). It is continuous throughout the region where the classical 2D molecule transits to two 2D classical atoms.

Different structural transitions are observed if we analyze the behavior of the minimum energy configuration as a function of the dielectric constant ( $\epsilon^*$ ). To this, we consider two positive charges (each one with  $Z = 3$ ) fixed at the points  $(1, 0, -1)$  and  $(-1, 0, -1)$  and six negative particles which are free to move in the  $xy$ -plane. For  $\epsilon^* = 1$  we are in region IV of the above. In Fig. 6 we show the distance of those six negative particles to the point  $(x, y, z) = (0, 0, 0)$  for the minimum energy configuration as a function of  $\epsilon^*$ . Eleven different regions are observed, of which we plot in Fig. 6 only the first ten of them. In region (I),  $1.0 < \epsilon^* < 1.054$ , the minimum energy configuration corresponds to the negative particles arranged in two triangles each one close to each positive charge (see Fig. 7(a)). When  $\epsilon^*$  is increased a structural transition takes place at  $\epsilon^* = 1.117$ . Up to this value of  $\epsilon^*$ , region (III), the configuration changes continuously and for  $\epsilon^* \rightarrow 1.225$  one of the negative particles becomes weakly bound and moves to infinity, i.e. it evaporates. After this value, region (IV), the minimum energy configuration changes continuously and again presents a structural transition, at  $\epsilon^* = 1.314$ , to a small region (V). This region goes up to  $\epsilon^* = 1.325$ , where a new structural transition takes place. Now, in the new region, region (VI), another

negative particle starts to become unbound when the value  $\epsilon^* = 1.492$  is reached. The minimum energy configuration is stable in the new region (VII) until the value  $\epsilon^* = 1.909$  and again changes its structure. After this point, again another particle starts to move away, region (VIII), and goes to infinity at  $\epsilon^* = 2.112$ . Up to this point, region (IX), only three particles remain bound until  $\epsilon^* = 3.000$ . In region(X)  $16.2 > \epsilon^* > 3.000$  only two particles remain, with each negative particle sitting almost on top of each of the positive charges in a symmetrical arrangement. Finally, when  $\epsilon^* > 16.2$  only one particle remains bounded. Unexpectedly, this negative particle stays in an asymmetric position, in this case at a distance  $r_i = 0.77$ . This fact can be confirmed by taking the minimum of the potential energy. In this case it presents a minimum at  $r_i = 0.77$  and a local maximum at  $r_i = 0$ , which corresponds to a symmetrical arrangement. The existence of region (X) shows that a bounded configuration can exist in a region where the condition  $Z_T \leq N - 1$  for  $N > 1$  is not satisfied.

#### IV. CONCLUSIONS

The molecule-atom transition and structural transitions were studied in a 2D model system of negative particles confined by a Coulomb potential of two positive impurity charges. This system presents a large variety of structural transitions as a function of its parameters, the distance between the impurity charges and the dielectric constant. As observed for a 2D like atom the 2D like molecule exhibits highly asymmetric ground state configurations which are related to broken symmetry states. However, the condition  $Z_T \leq N - 1$  for the existence of a bounded configuration is only satisfied if the positive particles are very close. Finally, our results show that a finite 2D system confined by a nonlinear potential presents a much larger wealth of structural transitions and new states as compared to the ones confined by parabolic potentials.

## ACKNOWLEDGMENTS

W. P. Ferreira, G. A. Farias, and H. A. Carmona are supported by the Brazilian Agencies, Fundação Cearense de Amparo à Pesquisa (FUNCAP), Brazilian National Research Council(CNPq) and The Ministry of Planning (FINEP). The work of F. M. Peeters is supported by the Flemish Science Foundation (FWO-VI), the EU-RTN network on 'Surface electrons on mesoscopic structures' and INTAS.

## REFERENCES

- [1] C. C. Grimes and G. Adams, Phys. Rev Lett. **42**, 795 (1979).
- [2] T. Ando, A. B. Flower and F. Stern, Rev. Mod. Phys. **54**, 437 (1982).
- [3] R. G. Clark, Phys. Scr. **T39**, 45 (1991).
- [4] D.H.E. Dubin and T.M. O'Neil, Rev. Mod. Phys. **71**, 87 (1999).
- [5] J.H. Chu and Lin I, Phys. Rev. Lett. **72**, 4009 (1994).
- [6] M. Saint Jean, C. Even, and C. Guthmann, Europhys. Lett. **55**, 54 (2001).
- [7] H. Aref and D. L. Vainchtein, Nature **392**, 769 (1998).
- [8] A. Isihara, Solid State Phys. **42**, 271 (1989).
- [9] V. M. Bedanov and F. M. Peeters, Phys. Rev. B **49**, 2667 (1994).
- [10] I. V. Schweigert, V. A. Schweigert, and F. M. Peeters, Phys. Rev. Lett. **82**, 5293 (1999).
- [11] M. Kong, B. Partoens, and F. M. Peeters, cond-mat/0106395 (to appear in Phys. Rev. E (2002)).
- [12] I. V. Schweigert, V. A. Schweigert, and F. M. Peeters, Phys. Rev. Lett. **84**, 4381 (2000).
- [13] G. A. Farias and F. M. Peeters, Solid State Commun. **100**, 711 (1996).
- [14] B. Partoens, V. A. Schweigert, and F. M. Peeters, Phys. Rev. Lett. **79**, 3980 (1997).

## FIGURES

FIG. 1. Schematic representation of the system considered in this paper.

FIG. 2. Distance  $r_i$  of the six negative particles to the point  $(x, y, z) = (0, 0, 0)$  for the minimum energy configuration as a function of the distance between the two positive particles  $x_p$ . Structural transitions are indicated by the vertical dotted lines.

FIG. 3. Typical configurations (and transitions) of the system in the different regions corresponding to Fig. 2.

FIG. 4. Distance of three negative particles related to each positive charge. Structural transitions are indicated by the vertical dotted lines.

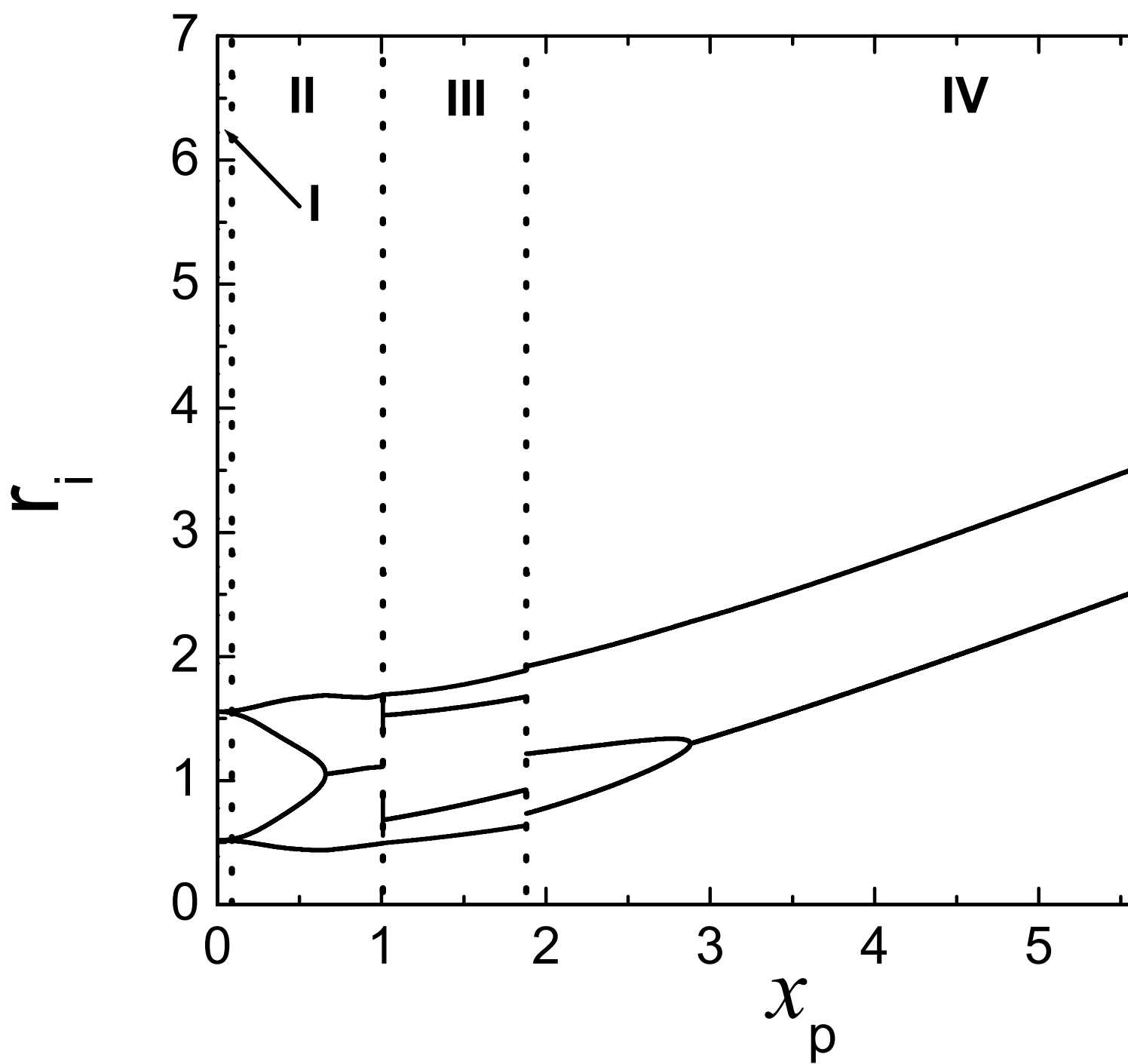
FIG. 5. The first derivative of the energy as a function of  $x_p$ . The inset is an enlargement of the small  $x_p$  region of the discontinuity of the first derivative. Structural transitions are indicated by the vertical dotted lines.

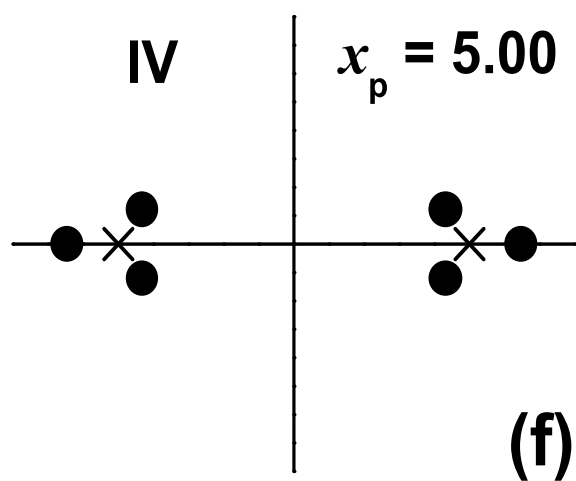
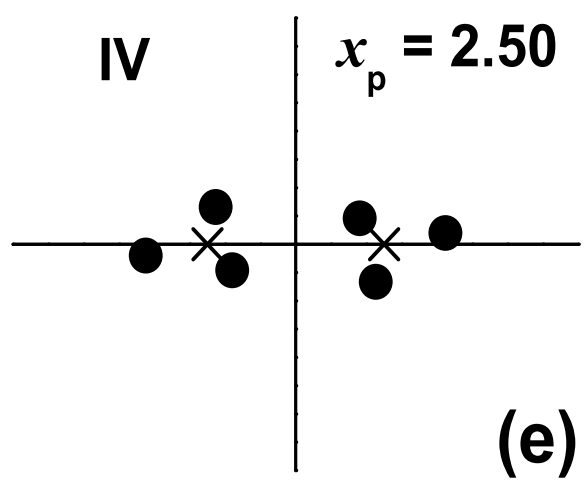
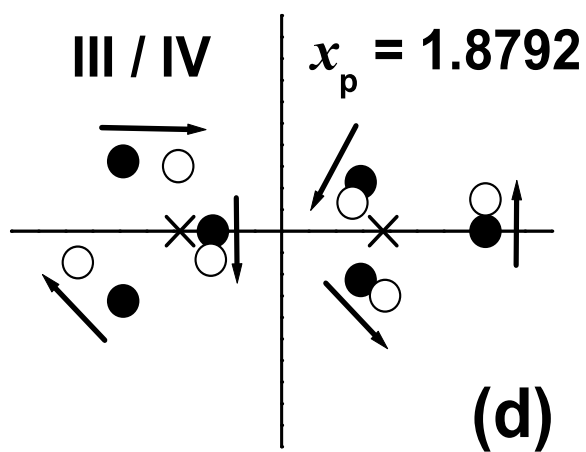
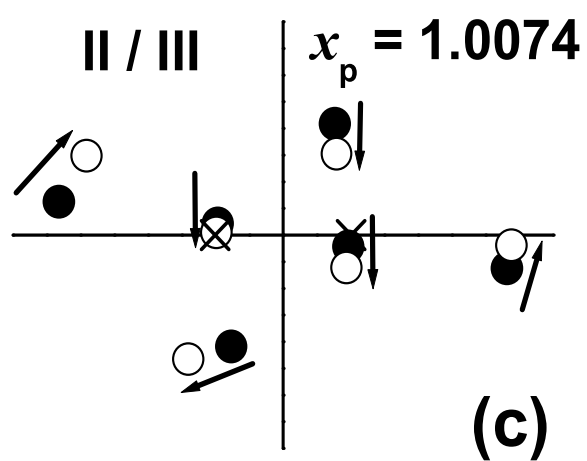
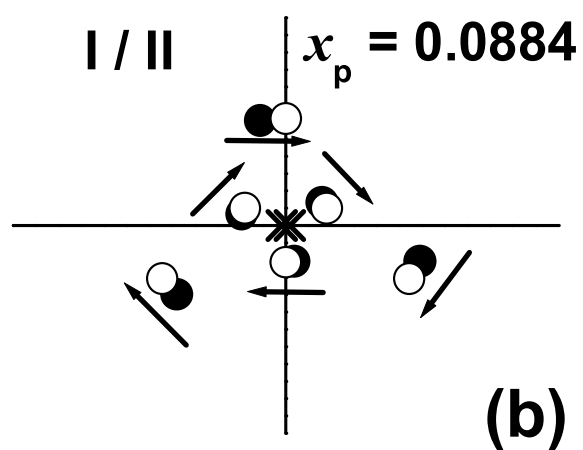
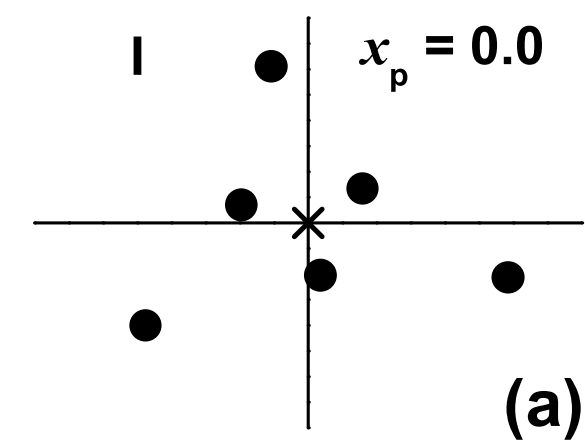
FIG. 6. Distance of six negative particles to the point  $(x, y, z) = (0, 0, 0)$  in the minimum energy configuration as a function of the logarithm of the dielectric constant  $\epsilon^*$ . The dashed lines indicate structural transitions while the vertical dotted lines correspond to the evaporation of a particle.

FIG. 7. Typical stable configurations of the ground state in different regions of  $\epsilon^*$ .

This figure "fig1.PNG" is available in "PNG" format from:

<http://arXiv.org/ps/cond-mat/0203137v1>





**Fig. 3**

